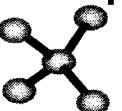


# Atomistic level simulation of the nanostructure properties

*Olga L. Lazarenkova<sup>1</sup>,*  
*Paul von Allmen<sup>1</sup>, Fabiano Oyafuso<sup>1</sup>, Seungwon Lee<sup>1</sup>,*  
*and Gerhard Klimeck<sup>1,2</sup>*

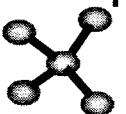
<sup>1</sup> - Jet Propulsion Laboratory, California Institute of Technology

<sup>2</sup> – School of Electrical Engineering, Purdue University



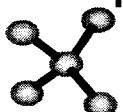
# Acknowledgements

- National Research Associateship Award at Jet Propulsion Laboratory for O.L.L.
- Funding was provided under grants from ARDA, ONR, JPL, and NASA



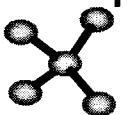
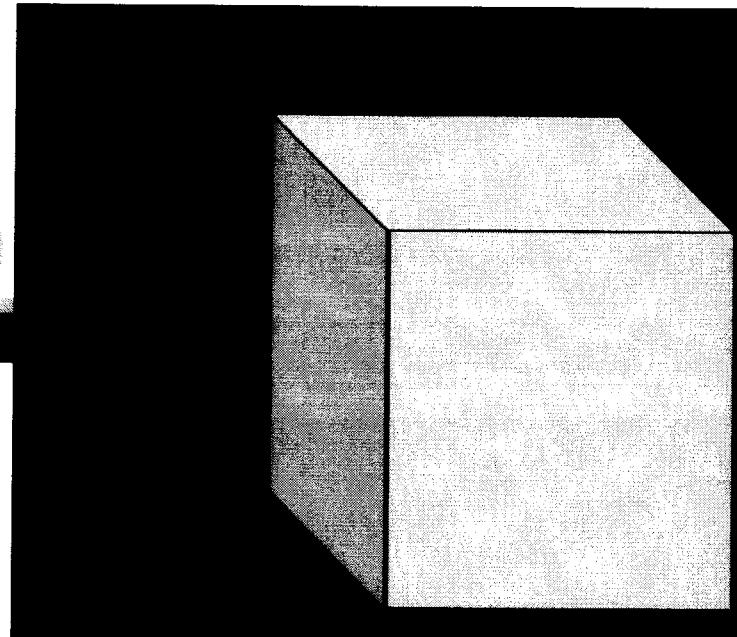
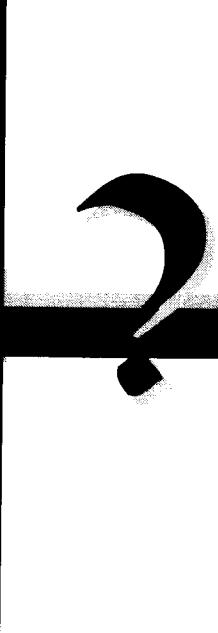
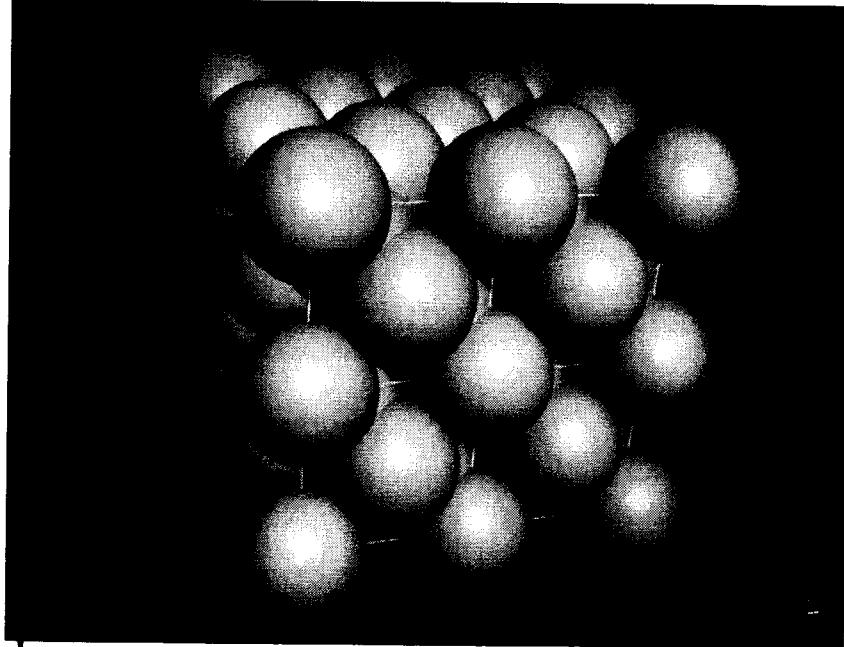
# Outline

- Motivation: Atomistic vs continuum treatment
- Vibration spectrum (phonons) in strained nanostructures
- Built-in strain distribution
  - Electronic spectrum in strained nanostructures
  - Strain penetration in the buffer
  - LO phonon red shift
- Conclusions



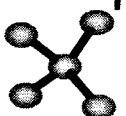
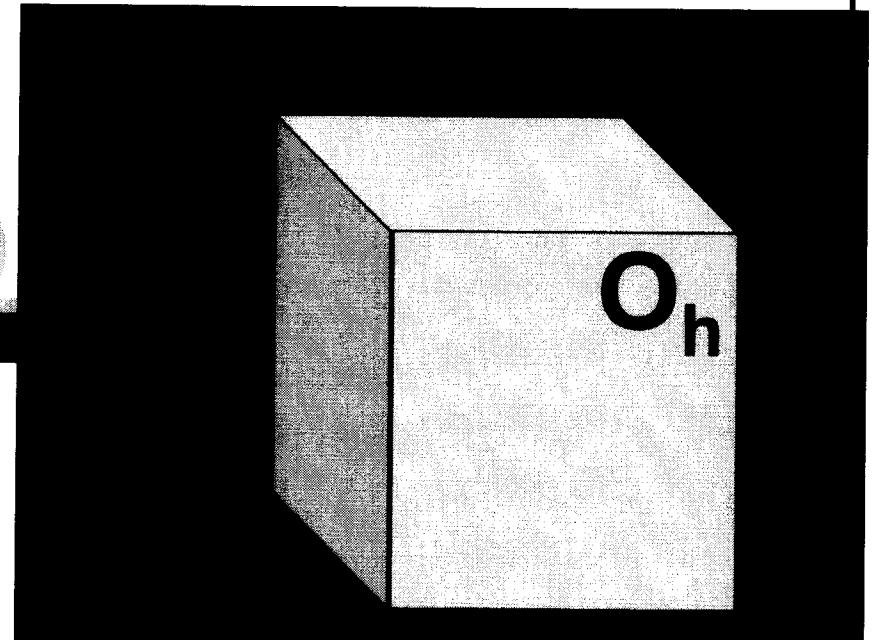
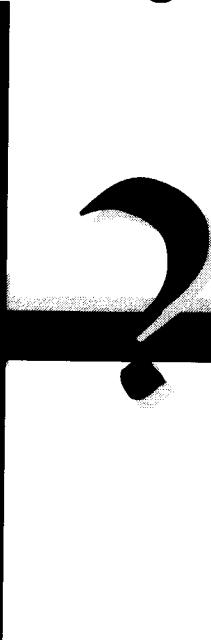
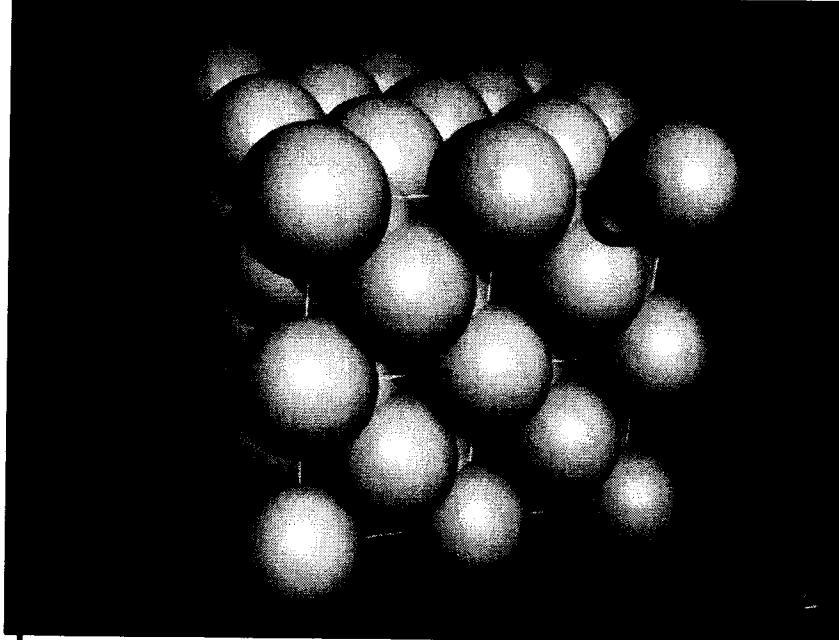
# Atomistic vs continuum treatment of nanostructures

- Uniform Si cluster



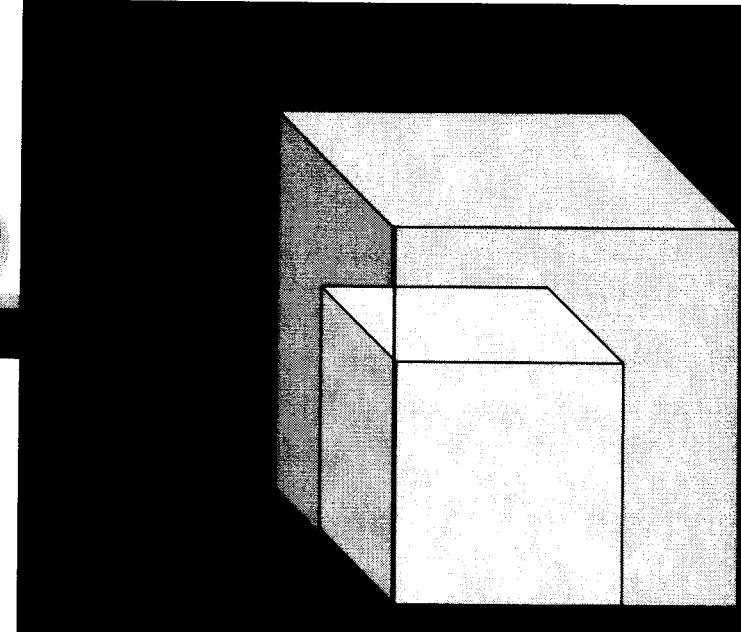
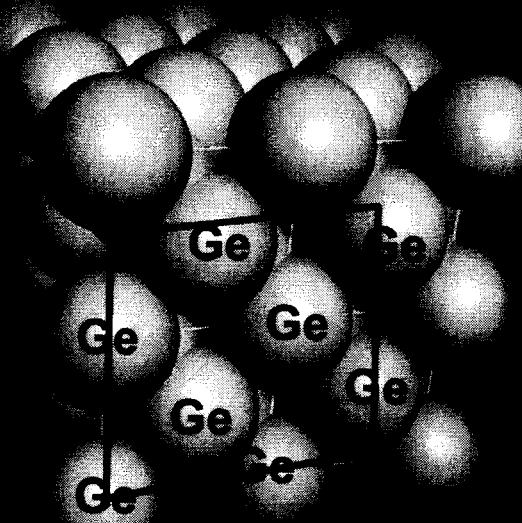
# Atomistic vs continuum treatment of nanostructures

- Uniform Si cluster
  - OK -- if # of atoms is large



# Atomistic vs continuum treatment of nanostructures

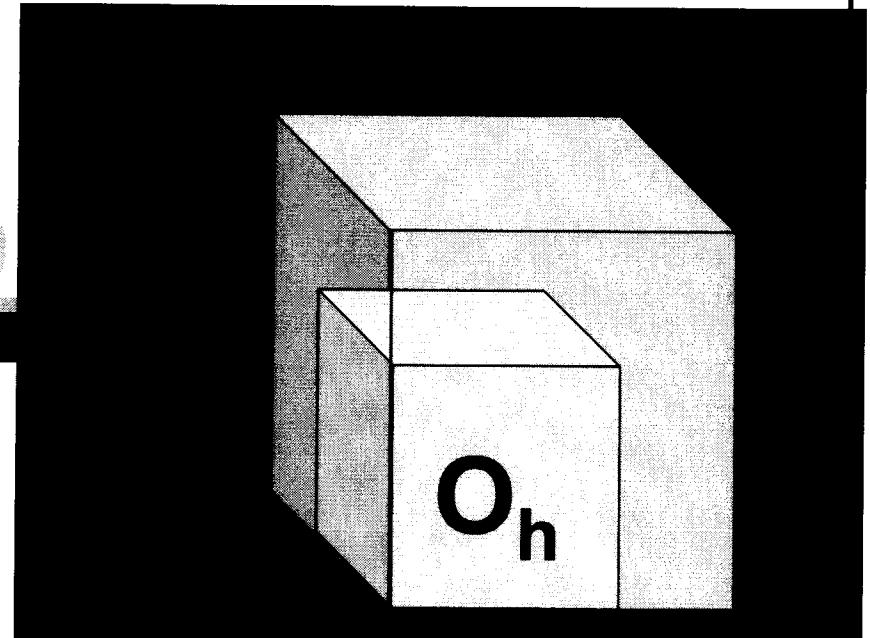
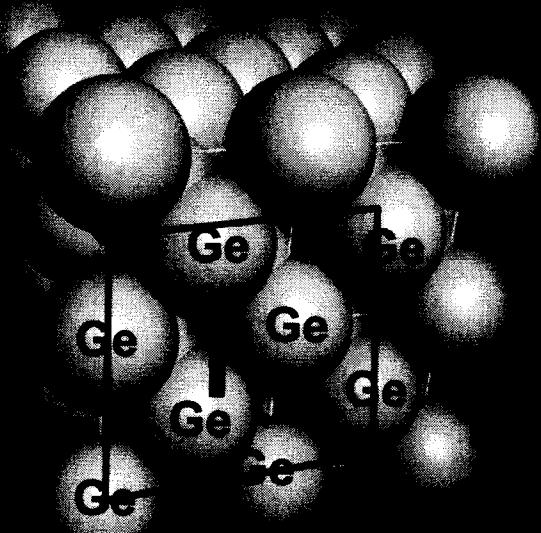
- Uniform Si cluster
  - OK -- if # of atoms is large



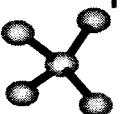
- Ge/Si nanostructure

# Atomistic vs continuum treatment of nanostructures

- **Uniform Si cluster**
  - OK -- if # of atoms is large

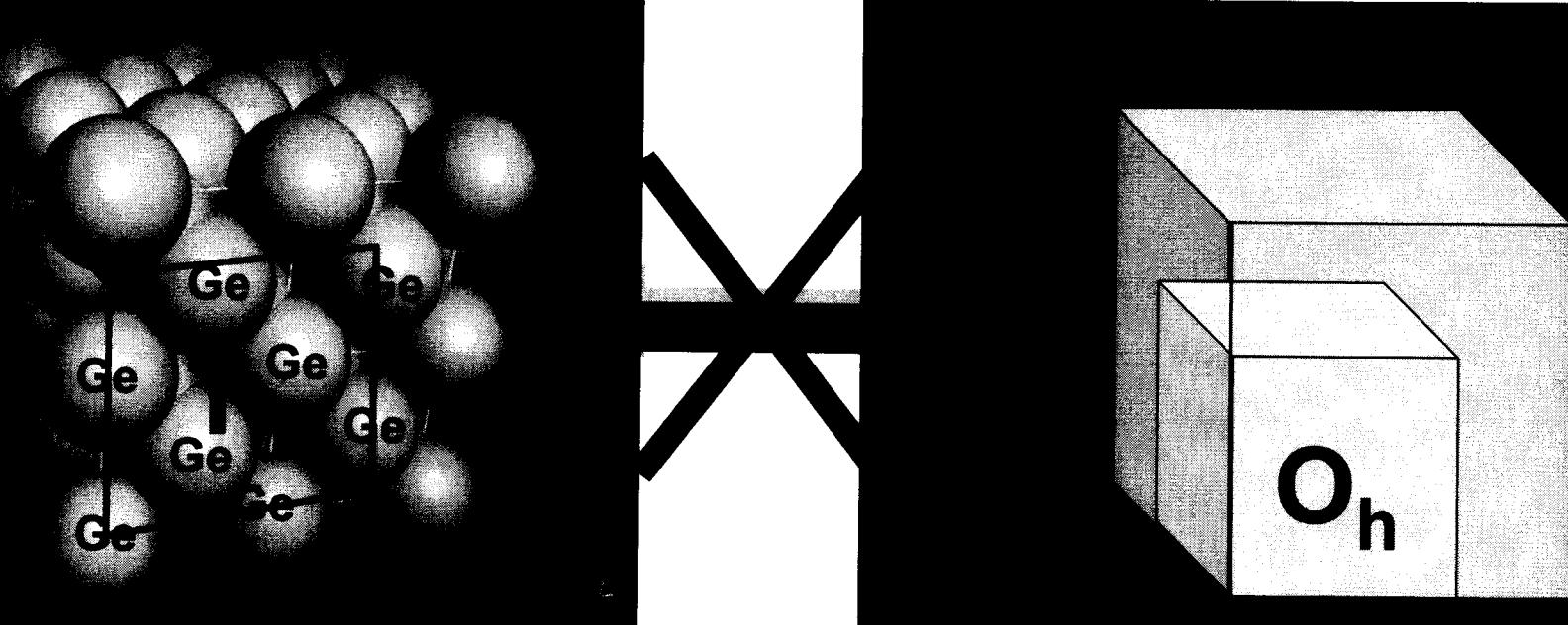


- **Ge/Si nanostructure**

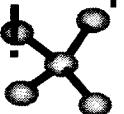


# Atomistic vs continuum treatment of nanostructures

- Uniform Si cluster
  - OK -- if # of atoms is large



- Ge/Si nanostructure
  - NO -- Different symmetry => different properties!!!

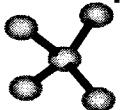


# Lattice vibrations – phonon spectrum

- Dynamical matrix elements

$$D_{\xi\xi}^{mn} = (M_m M_n)^{-1/2} \frac{\partial^2 \mathbf{E}}{\partial u_\xi(\mathbf{r}_m) \partial u_\xi(\mathbf{r}_n)}$$

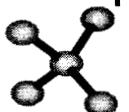
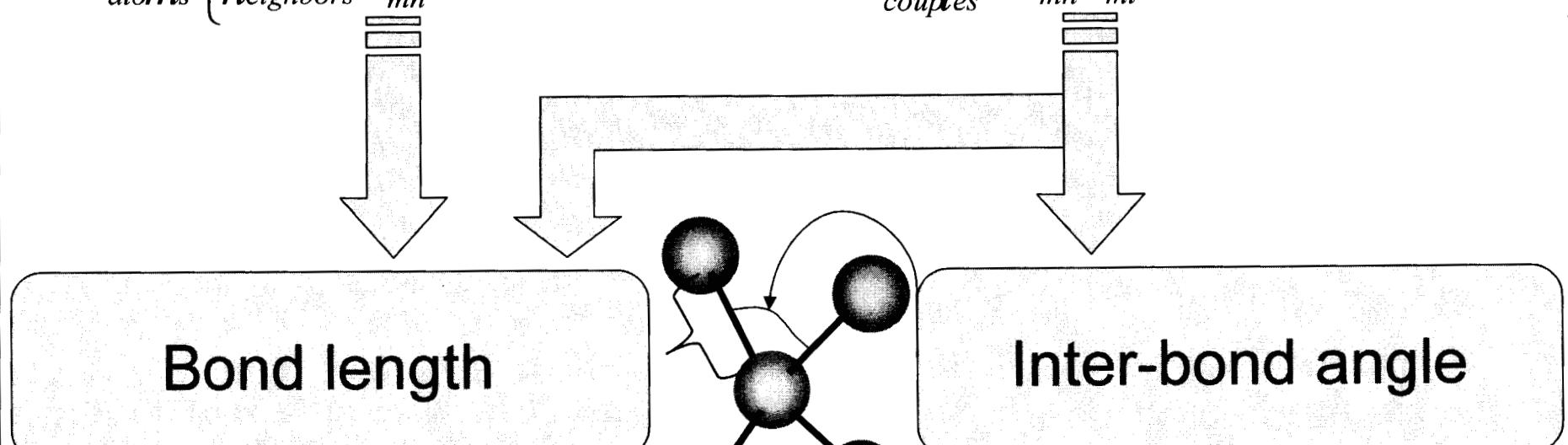
- $E$  – strain energy
- $m, n$  – indexes for atoms
- $M$  – atomic mass ( $10^{-26}$  kg)
- $\mathbf{r}_m, \mathbf{r}_n$  – coordinate of the  $m$ -th,  $n$ -th atom
- $\mathbf{u}=(u_x, u_y, u_z)$  – displacement of the atom
- $\xi$  --  $x, y$ , or  $z$  component of  $\mathbf{u}$



# Valence Force Field Model (VFFM)

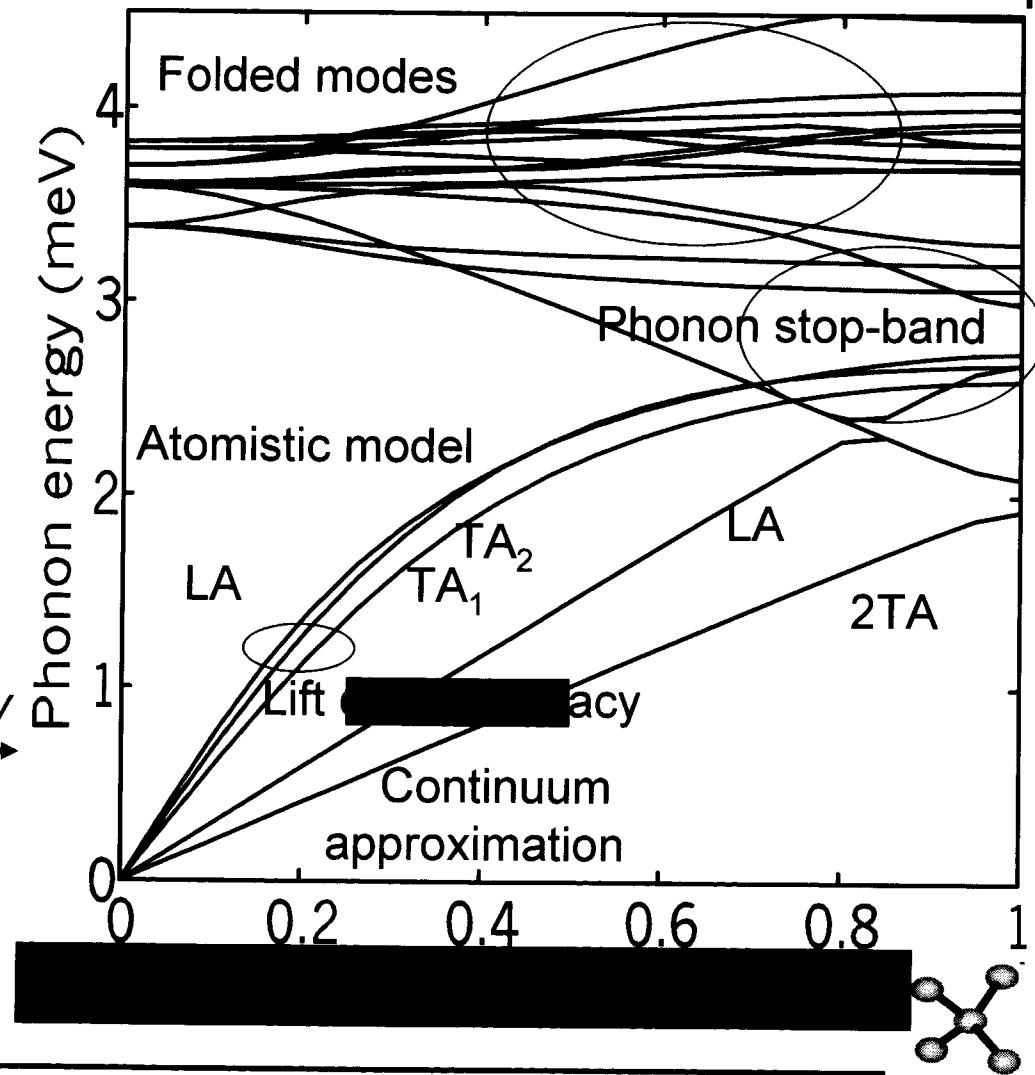
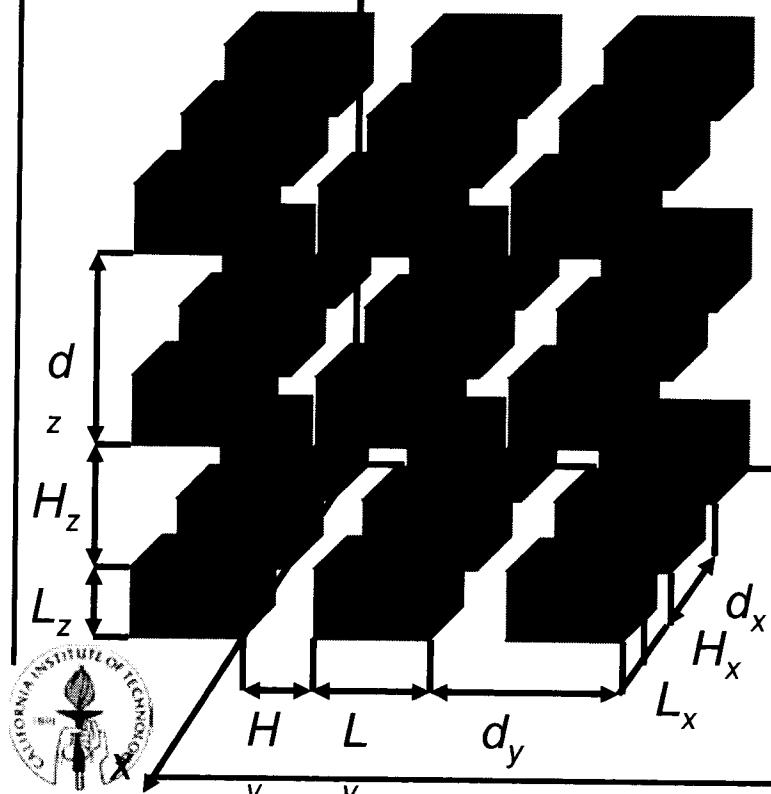
- Two-parameter nearest-neighbor Keating model

$$E = \frac{3}{8} \sum_{atoms} \left\{ \sum_{neighbors} \frac{\alpha_{mn}}{d_{mn}^2} (\mathbf{r}_{mn} \cdot \mathbf{r}_{mn} - \mathbf{d}_{mn} \cdot \mathbf{d}_{mn})^2 + \sum_{couples} \frac{\sqrt{\beta_{mn}\beta_{ml}}}{d_{mn}d_{ml}} (\mathbf{r}_{mn} \cdot \mathbf{r}_{ml} - \mathbf{d}_{mn} \cdot \mathbf{d}_{ml})^2 \right\}$$



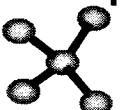
# Phonon spectrum of Ge/Si cubical Quantum Dot Crystal (QDC)

- $d_{xyz} = 5.5 \text{ nm}$
- $L_{xyz} = 2.5 \text{ nm}$



# Atomistic vs continuum treatment of phonons in nanostructures

	Continuum	Atomistic
Sound velocity	~average of the constituent materials	Energy-dependent
Lift of degeneracy	no	yes
Folding modes	yes	yes
Stop-band	no	yes

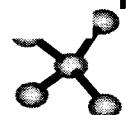
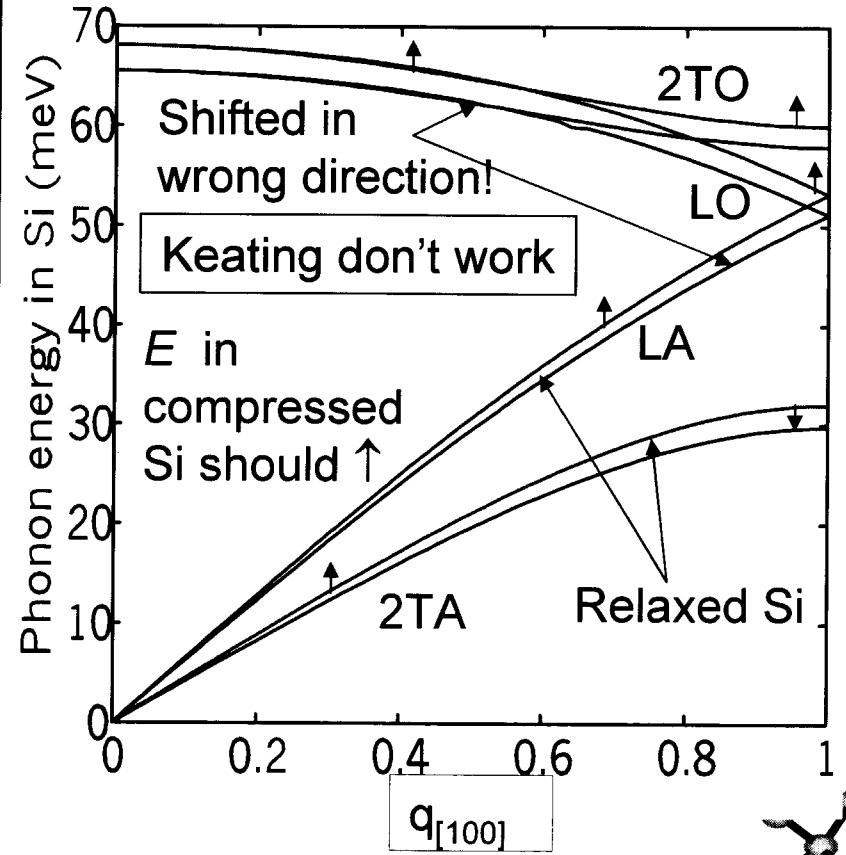


# Effect of strain on phonon spectrum

- Ge/Si 4% lattice mismatch
- Grüneisen coefficient

$\gamma_{\text{Si}}$	Keating	Exp.
$\gamma_{\text{TA}}^{\Gamma}$	-1.41	0.325
$\gamma_{\text{LA}}^{\Gamma}$	-0.96	1.110
$\gamma_{\text{TA}}^X$	-1.13	-1.4
$\gamma_{\text{LA}}^X$	-0.62	1.03
$\gamma_{\text{LTO}}^{\Gamma}$	-0.61	0.98-1.02
$\gamma_{\text{TO}}^X$	-0.56	1.5
$\gamma_{\text{LO}}^X$	-0.62	1.03

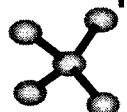
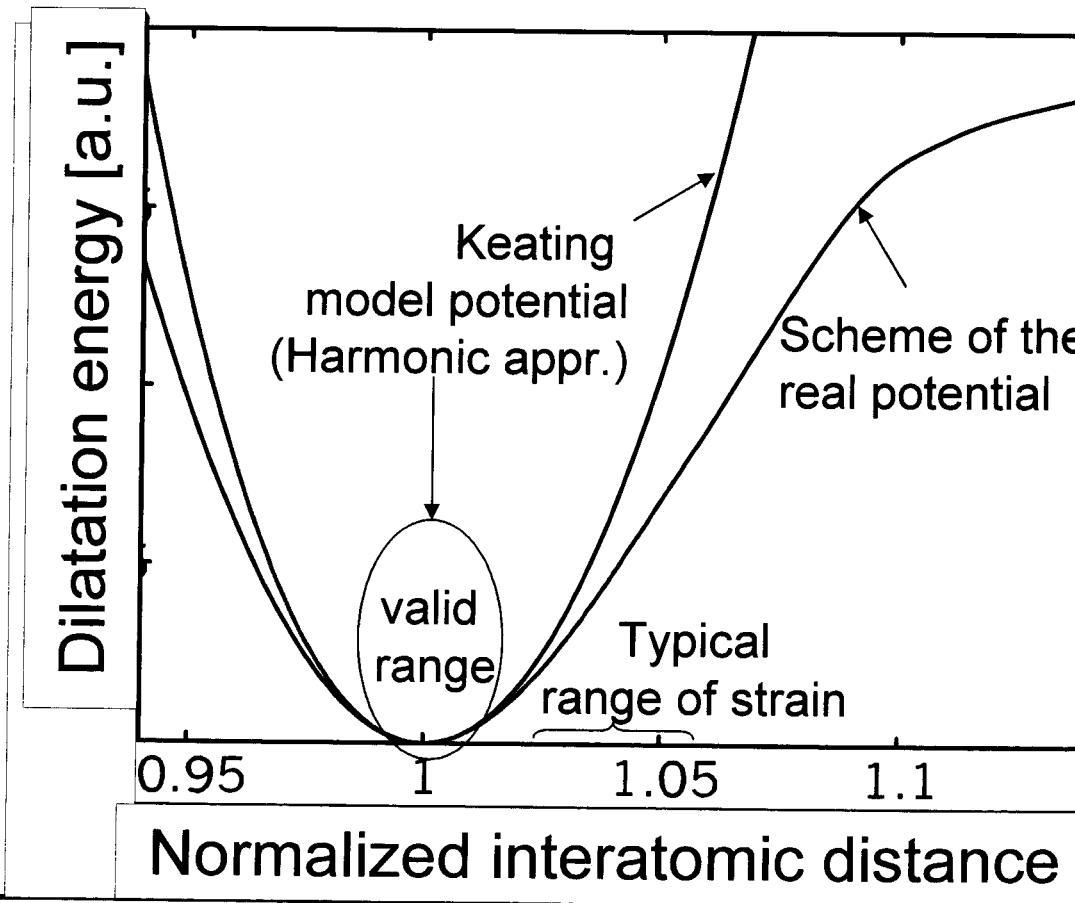
$$\gamma_i = - \frac{V}{\omega_i} \frac{d\omega_i}{dV}$$



# Interatomic potential

- Dynamical matrix elements

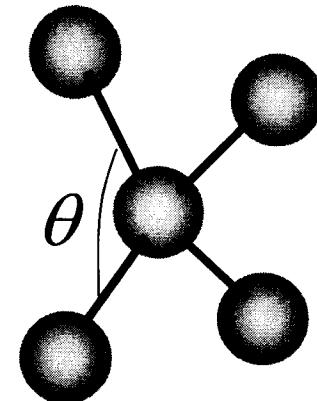
$$D_{\xi\xi}^{mn} = (M_m M_n)^{-1/2} \frac{\partial^2 E}{\partial u_\xi(\mathbf{r}_m) \partial u_\xi(\mathbf{r}_n)}$$



# Anharmonicity corrections

- Valence-Force Field constants

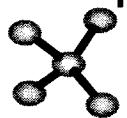
$$\alpha = \alpha_0 \left[ 1 - A \frac{\left( r_{mn}^2 - d_{mn}^2 \right)}{d_{mn}^2} \right]$$



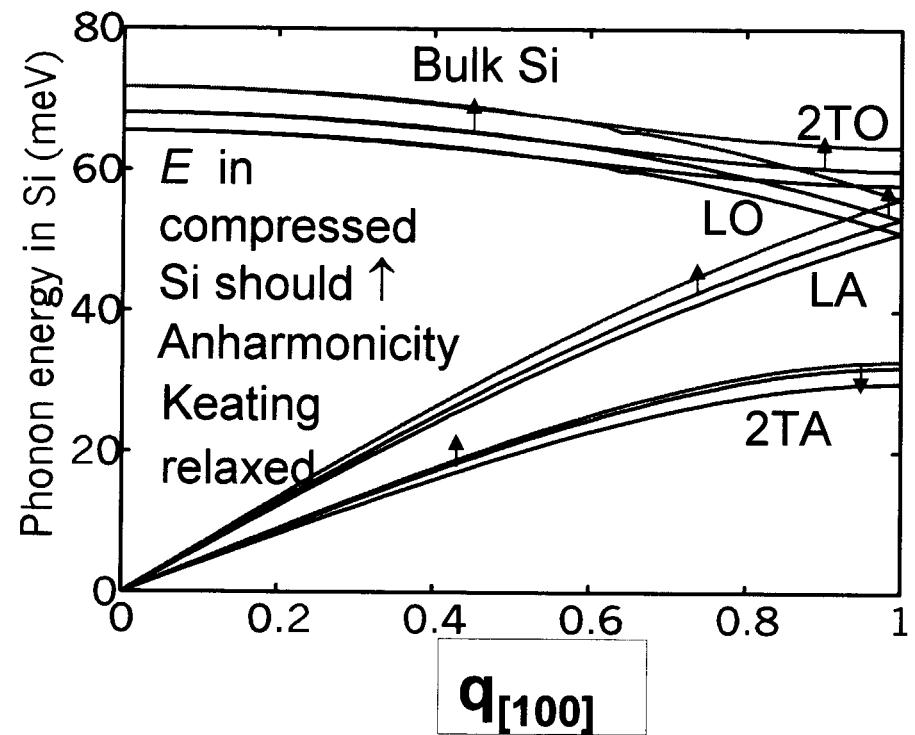
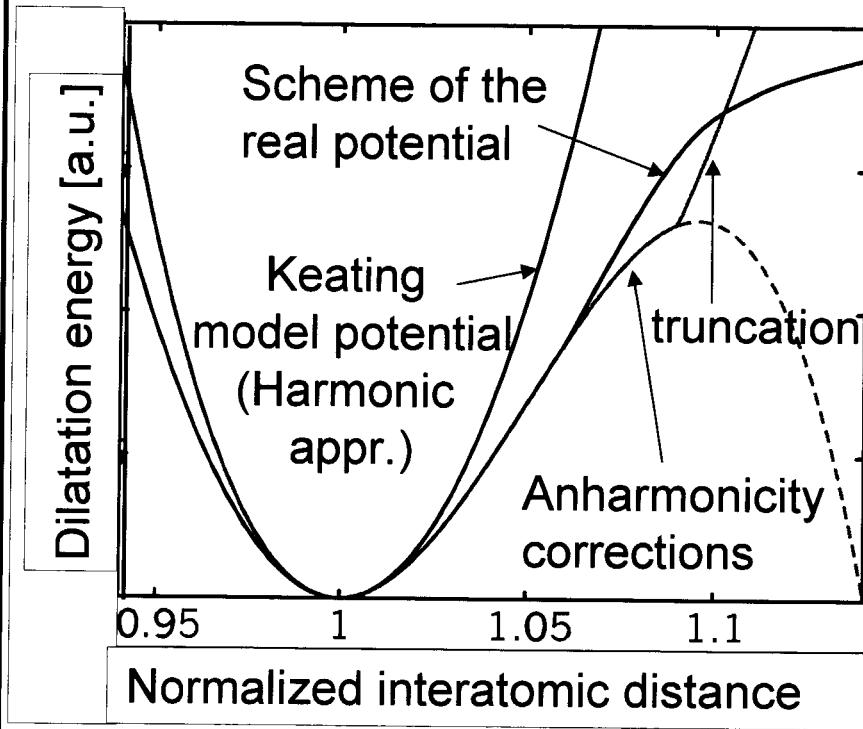
$$\beta = \beta_0 \times \left[ 1 - C \frac{r_{mn}r_{ml} - d_{mn}d_{ml}}{d_{mn}d_{ml}} \right] \times [1 - B(\cos \theta - \cos \theta_0)]$$

- A,C – fit to the Grüneisen coefficients
- B – found from the shear deformation parameter

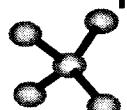
$$a_s = 1 - \frac{2B\beta_0}{3(\alpha_0 + \beta_0)}$$



# Phonons in strained bulk material

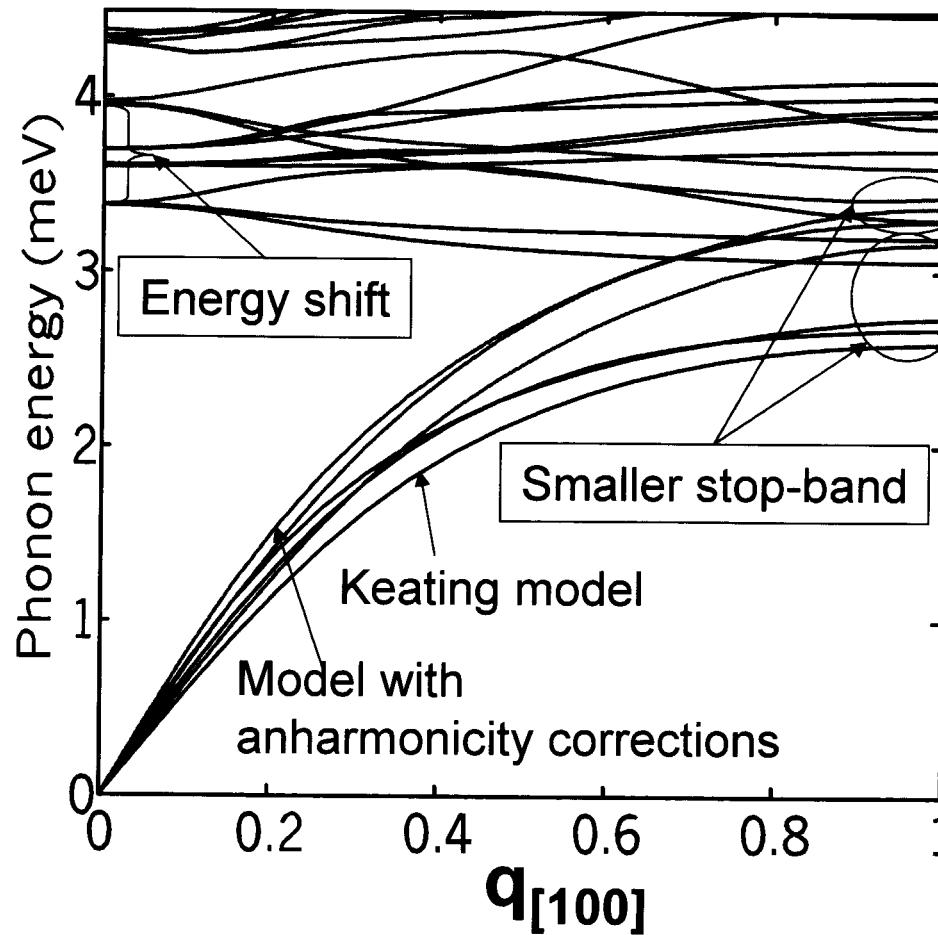


	Keating (harmonic appr.)	Anharmonicity corrections
Relaxed bulk	yes	yes
Strained mat.	no	yes



# Phonon dispersion of relaxed Ge/Si cubical QDC

- $d_{xyz} = 5.5 \text{ nm}$ ,  $L_{xyz} = 2.5 \text{ nm}$

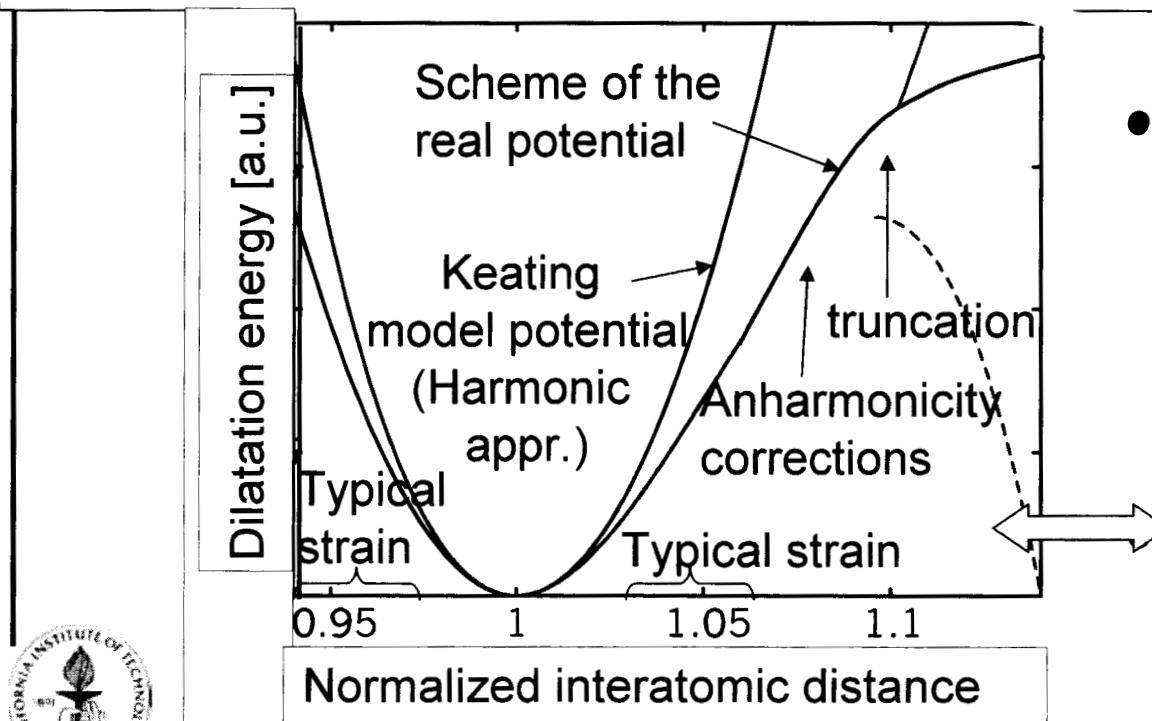


Because of the  
**built-in strain**

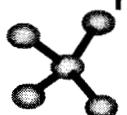
# Effect of the anharmonicity on strain distribution

- Minimize the total strain energy in the structure

$$E = \frac{3}{8} \sum_{atoms} \left\{ \sum_{neighbors} \frac{\alpha_{mn}}{d_{mn}^2} (\mathbf{r}_{mn} \cdot \mathbf{r}_{mn} - \mathbf{d}_{mn} \cdot \mathbf{d}_{mn})^2 + \sum_{couples} \frac{\sqrt{\beta_{mn}\beta_{ml}}}{d_{mn}d_{ml}} (\mathbf{r}_{mn} \cdot \mathbf{r}_{ml} - \mathbf{d}_{mn} \cdot \mathbf{d}_{ml})^2 \right\}$$



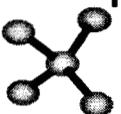
- Valence-force field coefficients depend on strain
- ↔
- anharmonicity corrections



# Ultra-thin epitaxial layers

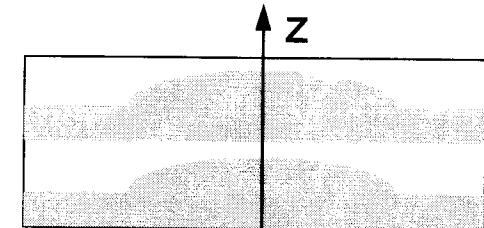
Structure	Size		Hydrostatical strain (%)			Biaxial strain (%)		
	layer	cap	K	A	$\delta(\%)$	K	A	$\delta(\%)$
InAs/GaAs SQW	2ML	5ML	-2.97	-2.59	19.9	-3.71	-4.10	-9.4
InAs/GaAs MQW	1ML	30nm	-2.87	-2.33	23.5	-3.81	-4.38	-13.0
GaAs/InAs SQB	2ML	5ML	6.54	4.30	-17.7	3.72	2.90	28.3

- Biaxial compression – increased with anharmonicity
- Hydrostatic compr. – reduced with anharmonicity

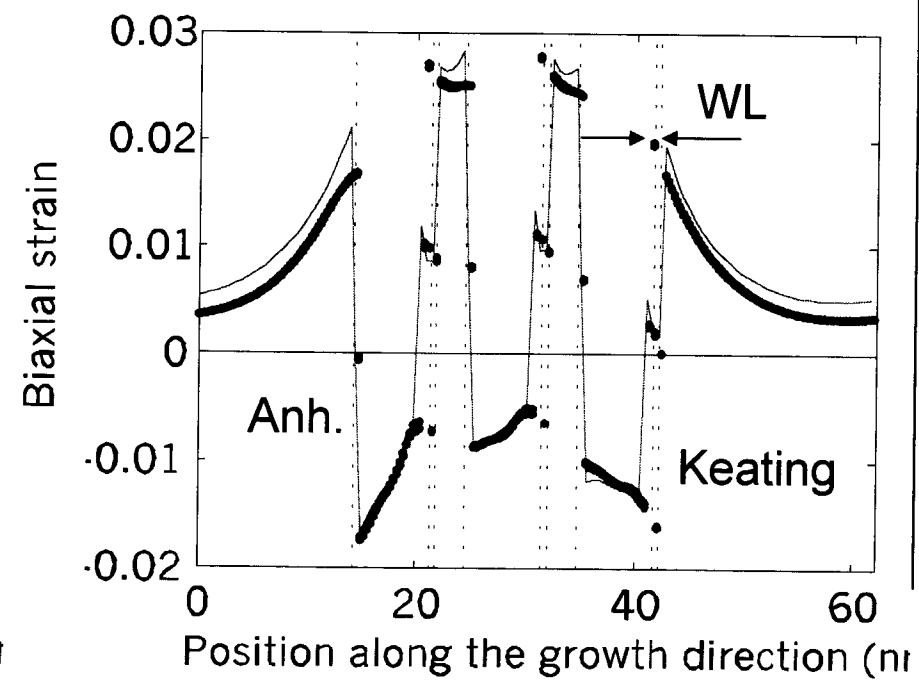
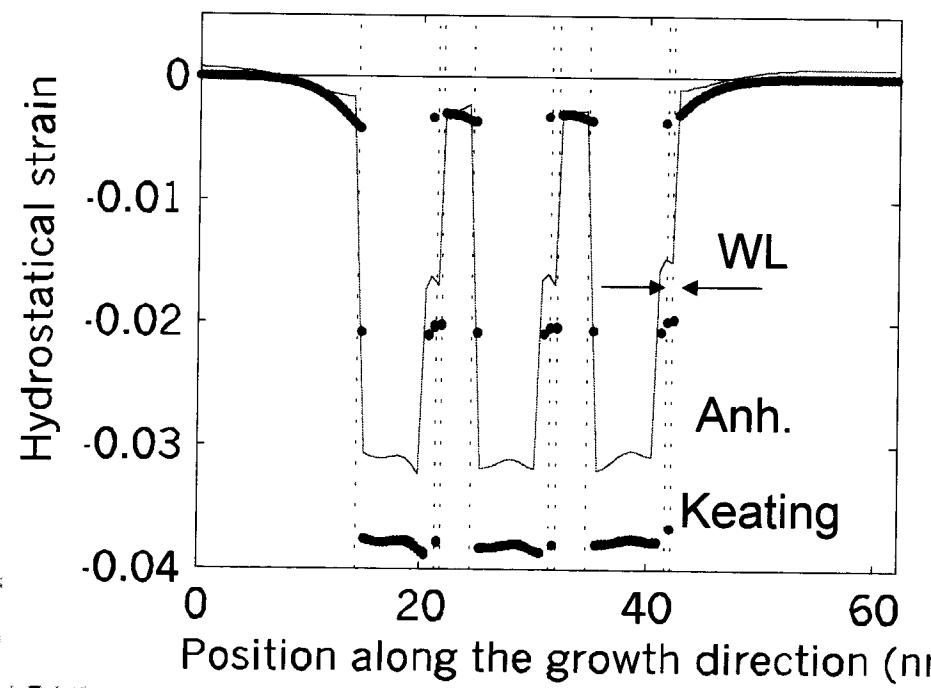


# Built-in strain in InAs/GaAs QDC

- InAs/GaAs dome QDC
  - Dome QD:  $L_{xy} = 20 \text{ nm}$ ,  $H_z = 7 \text{ nm}$
  - Wetting layer:  $W = 0.7 \text{ nm}$
  - Periodicity:  $D_{xy} = 60 \text{ nm}$ ,  $D_z = 10 \text{ nm}$



S. Ghosh, B. Kochman,  
and P. Bhattacharya,  
APL 76, 2571 (2000).

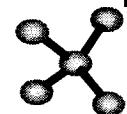
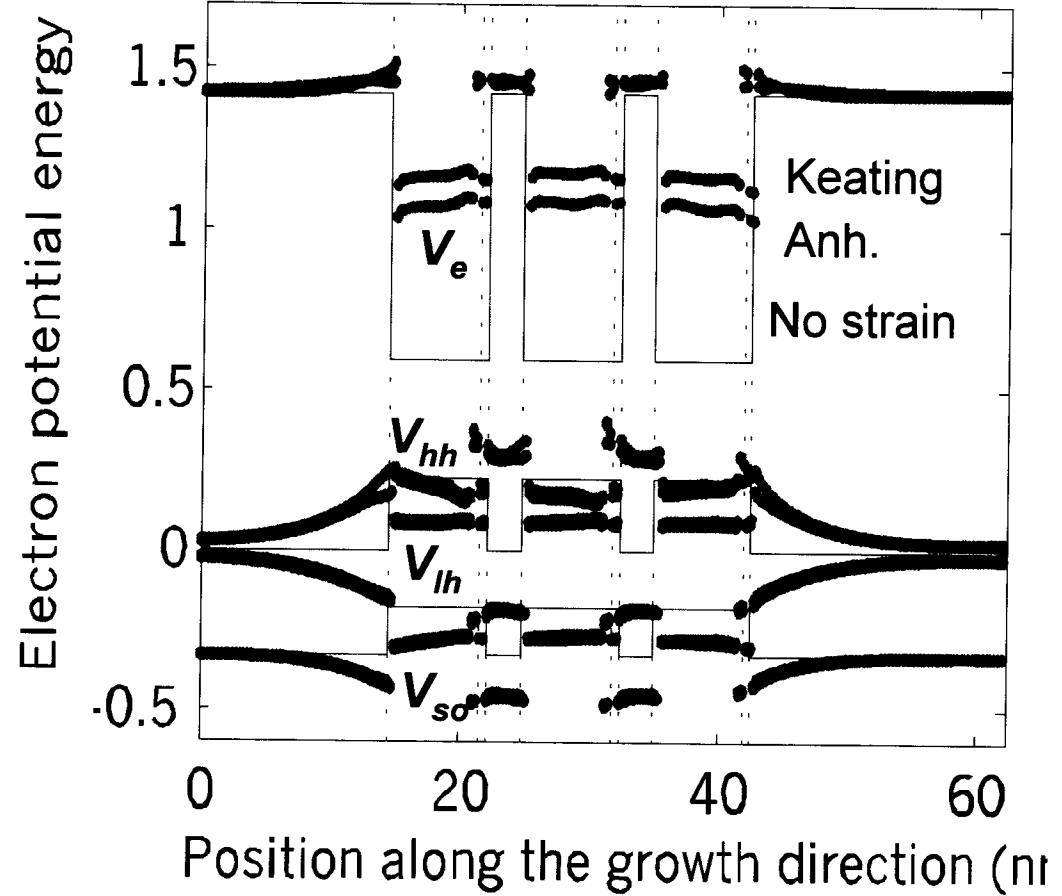


# Band offsets in InAs/GaAs nanostructures

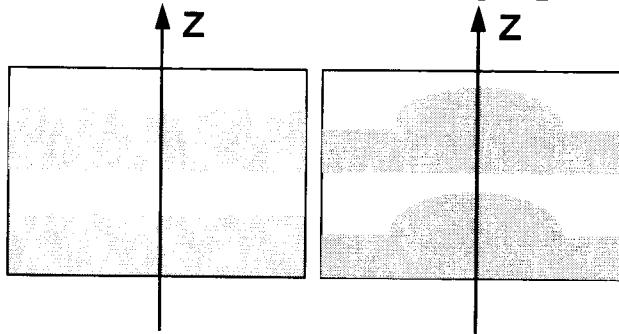
- Band offset in conductance band (meV) is very sensitive to the hydrostatic strain

Keating	Anh.	Exp.
242.0	347.0	$341 \pm 30$

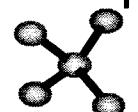
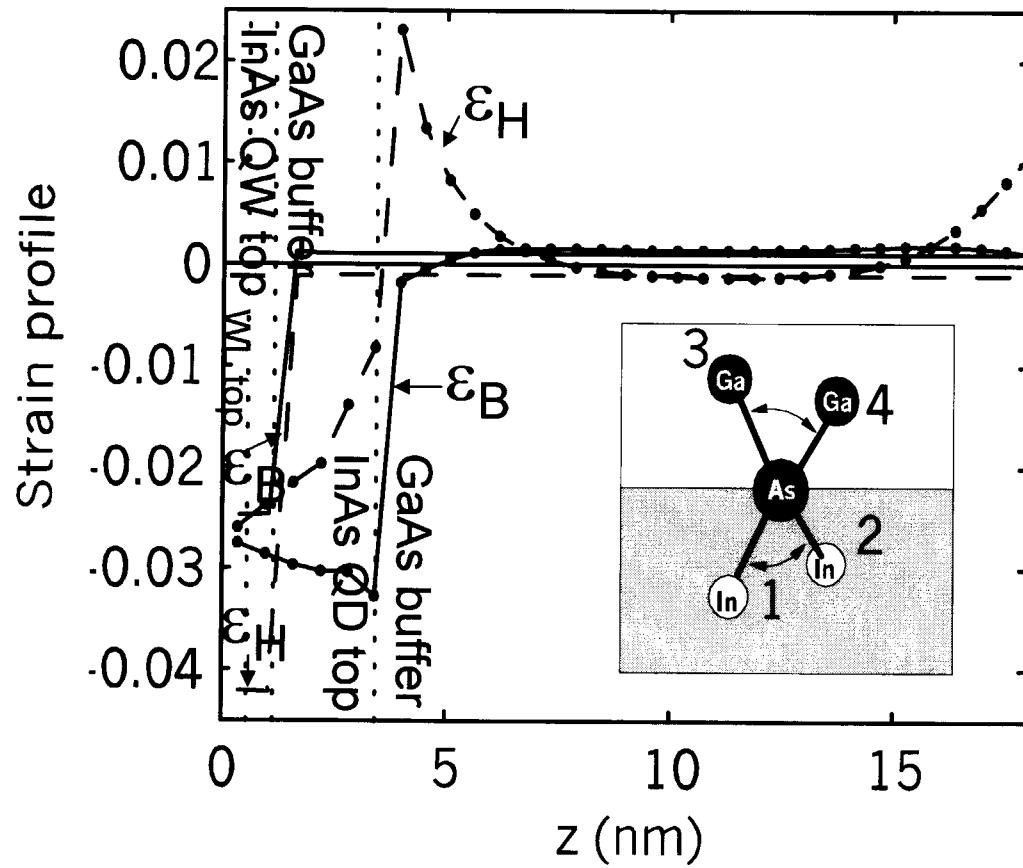
- Large biaxial strain => type II valence band alignment



# Penetration of strain into GaAs buffer of InAs/GaAs periodical structures

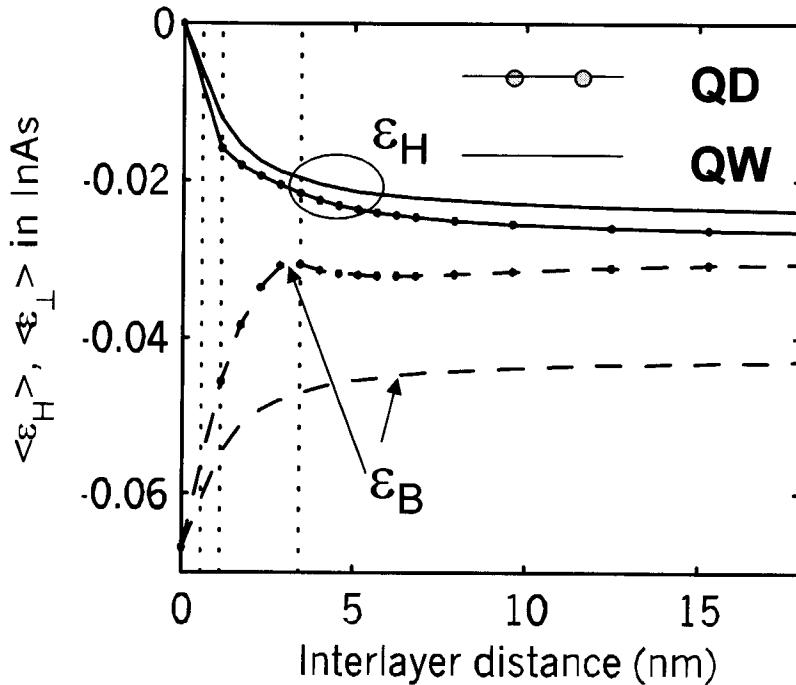


- Bond angle deformation results in penetration of
  - Hydrostatic
  - Biaxialstrain in both InAs and GaAs

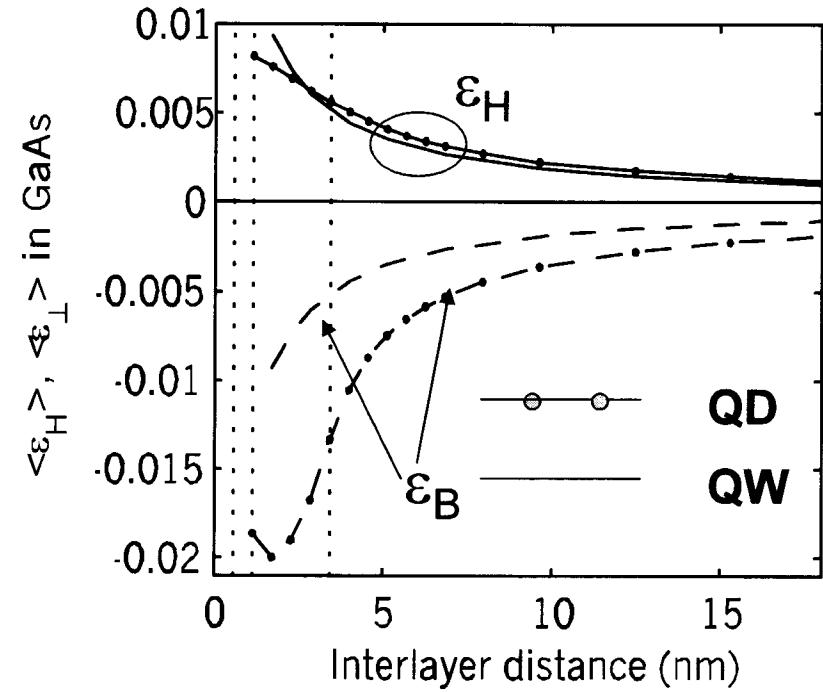


# Average strain depends on interlayer distance

- InAs

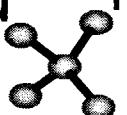


- GaAs



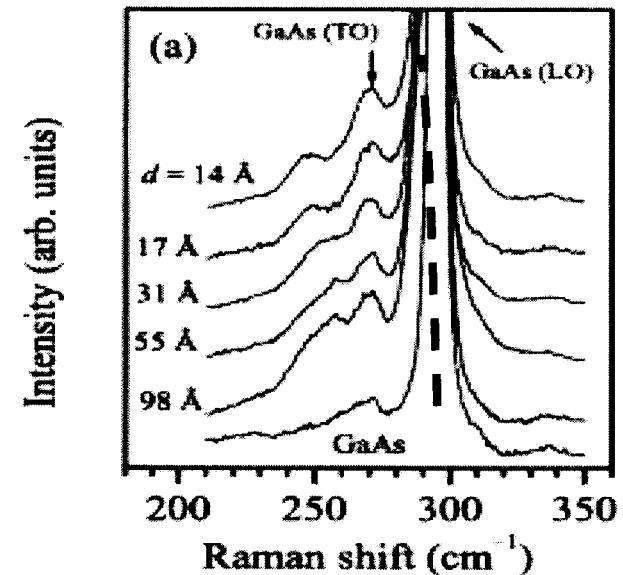
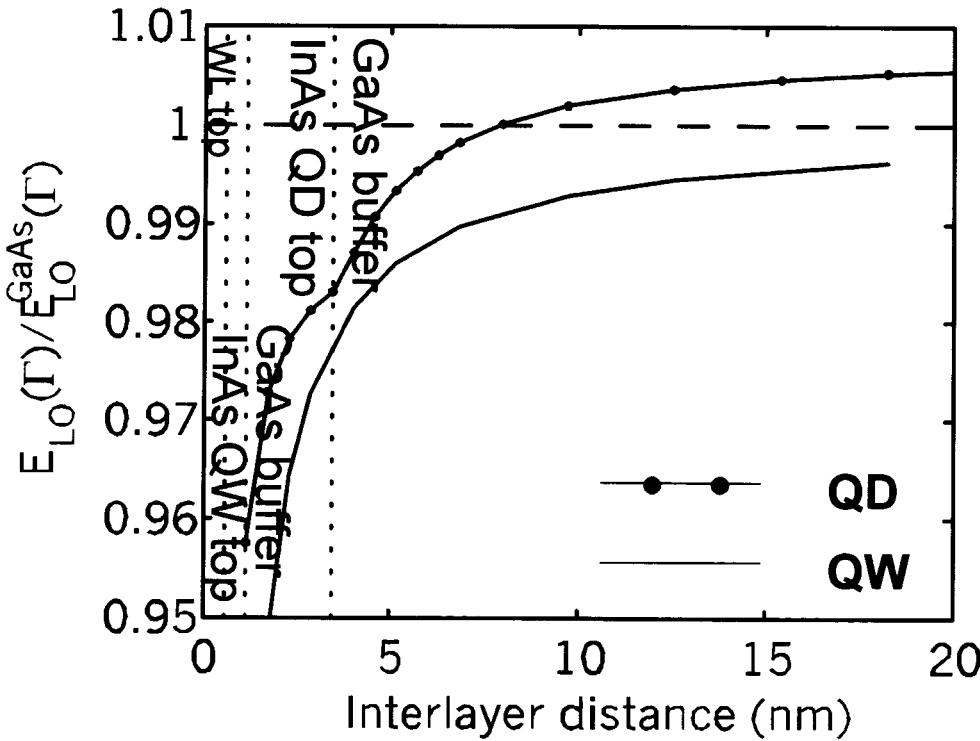
- Pure biaxial strain only at 0 separation

- GaAs adjacent to InAs always strained

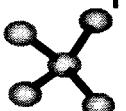


# Red Raman shift at small separation

- Strain => red shift
- LO Confinement => blue shift



J. Ibanez, A Patane, M. Henini, L. Eaves, S. Hernandez, R. Cusco, L. Artus, Yu.L. Musikhin, and P.N. Broukov,  
APL 83, 3096 (2003).



# Conclusions

- Only atomistic treatment can reproduce all properties of nanostructures
- Anharmonicity of the interatomic potential strongly affects
  - Strain distribution
  - Vibration properties
  - Electronic spectrum
- NEMO3D is a powerful NanoElectronic MOdeling tool for the simulation of electron and phonon properties of nanostructures with up to several million atoms

